Transport Properties of the One Dimensional Ferromagnetic Kondo Lattice Model : A Qualitative Approach to Oxide Manganites

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The transport properties of the ferromagnetic Kondo lattice model in one dimension are studied via bosonization methods. The antiferromagnetic fluctuations, which normally appear because of the RKKY interactions, are explicitly taken into account as a direct exchange between the "core" spins. It is shown that in the paramagnetic regime with the local antiferromagnetic fluctuations, the resistivity decays exponentially as the temperature increases while in the ferromagnetic regime the system is an almost perfect conductor. The effect of a weak applied field is discussed to be reduced to the case of the ferromagnetic state leading to band splitting. The qualitative relevance of the results for the problem of the Oxide Manganites is emphasized.

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The Kondo lattice model fundamentally captures the physics of heavy electron systems (e.g. Uranium or Cerium compounds). Therefore the efforts to study it have been intensive for a long time. One route to the full understanding has been the study of the one-dimensional(1D) analogue due to well developed techniques that can be used [1]. More recently another class of materials, where a ferromagnetic version of the Kondo lattice model is expected to be the starting point, has been extensively studied. These are the manganite oxides of the form $Ln_{1-x}A_xMnO_3$ where Ln is a lanthanide and A is an alkaline-earth element, which possess a very rich phase diagram [2]. As a function of doping there are regions of ferromagnetic (FM), antiferromagnetic (AFM) as well as charge ordering. Moreover there is an almost insulating state above the FM critical temperature, where a huge increase in resistivity is observed and becomes even more dramatic with the application of an external field. This phenomenon is termed as "Colossal Magnetoresistance" (CMR). The FM order can be explained by the double exchange mechanism [3]. This mechanism though, is clearly not enough to explain the CMR [4] and other possibilities have been proposed - e.g. the relevance of Jahn-Teller distortion [5], the effect of AFM fluctuations or localization due to randomness etc. [6] - to explain the phenomenon. A deep understanding of the relevant electronic models is vital and the FM Kondo Model, especially in 1D case, is the first candidate in this direction as well.

Recently Monte Carlo calculations have demonstrated the potential of a very rich phase diagram of the FM Kondo Hamiltonian [7]. At low temperatures and as a function of doping and interaction strength, regimes with paramagnetic, FM, incommensurate correlations and also phase separation between undoped AFM and hole-rich FM regions have been observed. The similarities in the behavior of the 1D system with a higher dimensional one, are also emphasized.

In this work a reversed question is examined: given the local spin configuration, what the consequences for the transport properties are. The starting point is the following Hamiltonian :

$$H = -t \sum_{<i,j>,\alpha} c^{\dagger}_{i,\alpha} c_{j,\alpha} + h.c. - J_H \sum_{i,\alpha,\beta} c^{\dagger}_{i,\alpha} \sigma_{\alpha,\beta} c_{i,\beta} \cdot \vec{S}_i. \tag{1}$$

In the "language" of the CMR problem, the first term represents the e_g electron hopping between nearest-neighbor Mn ions at sites i and j. The second term is the Hund's rule coupling between the localized spins $\vec{S}_j$ (the t_{2g} singly occupied orbitals with S=3/2) and the mobile e_g electron at the same site. A direct AFM exchange between the nearest "core" spins $H_{AFM} = J_{AFM} \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j$ can be added to ensure the presence of the AFM fluctuations. This effect is present and important at half filling, even in the absence of the direct exchange term, through the RKKY interactions. The latter are the effective interactions between the "core" spins once the fermionic degrees of freedom are integrated out. However the need of this direct exchange term has to be emphasized on pure experimental grounds since AFM short range order has been observed by neutron scattering experiments on $La_{1.2}Sr_{1.8}Mn_2O_7$ (which is a compound of reduced dimensionality) [9] in addition to the fact that regimes of AFM ordering are adjacent to the FM as a function of doping in the experimental phase diagram. Moreover the direct exchange interaction is always present [8] and can be crucial for the formation of localized spin polarons, and for the insulating behavior in the paramagnetic phase. Thus, we take into account this direct AFM interaction explicitly, and investigate the effects of local AFM fluctuations. Following the experimental observation [9], we assume $J_{AFM} \ll J_H$. The

opposite limit $J_{AFM} \gg J_H$, the case of which was studied before in another context, gives a quite different physics [10].

The approach followed in this Letter is the abelian and non-abelian bosonization [11] of the charge and spin degrees of freedom of the conduction electrons respectively, with the coherent path integral method for the localized spins. Then the effective action reads :

$$S = \int dxd\tau[v(\partial_x\phi_c)^2 + \frac{1}{v}(\partial_\tau\phi_c)^2] + S_{WZW}(g) + J_{Hr}\int dxd\tau(\vec{J_L} + \vec{J_R} + e^{i2k_Fx}\mathrm{Tr}(g\vec{\sigma})e^{i\sqrt{2\pi}\phi_c} + h.c.)\cdot\vec{S_i} + S_{AFM}, \quad (2)$$

where ϕ_c is the boson field for the charge degrees of freedom, $\vec{J_L}$ and $\vec{J_R}$ are the spin current operators which satisfy level-1 SU(2) Kac-Moody algebra, v is the velocity which is the same for the charge and spin degrees of freedom, g(x) is a representation of SU(2) and S_{WZW} is the Wess-Zumino-Witten action given by [12]:

$$S_{WZW} = -\frac{1}{16\pi}\int d^2x\mathrm{Tr}(\partial_\mu g^{-1}\partial_\mu g) + \frac{i}{24\pi}\int_0^\infty d\xi\int d^2x\epsilon^{\alpha\beta\gamma}\mathrm{Tr}(g^{-1}\partial_\alpha g g^{-1}\partial_\beta g g^{-1}\partial_\gamma g). \quad (3)$$

S_{AFM} is the action for the localized spins obtained by applying the coherent path integral method to H_{AFM} [13].

In the absence of a direct exchange term, at half-filling, the J_{Hr} term (which comes from the renormalization of J_H) is marginally irrelevant and scales to zero. On the other hand the RKKY interaction becomes important and gives rise to a dispersion of localized spins [14,15]. The configuration of the localized spins can be parametrized in the case of general filling as :

$$\vec{S_j} = S(\vec{l_j} + \sqrt{1 - {l_j}^2}\vec{m_j}), \quad (4)$$

with j enumerating the cites and $\vec{l}\cdot\vec{m} = 0$ where $\vec{l}$ is the fast variable whereas a unit vector $\vec{m}$ is the slow one.

Paramagnetic regime: We first consider the effects of local AFM fluctuations in the paramagnetic (PM) state. We assume $J_{AFM} \gg J_H^2/v$. This condition ensures that the direct AFM correlation between localized spins dominates over the $2k_F$ RKKY correlation. This situation is actually realized in the systems with the 2D layered structure, $La_{1.2}Sr_{1.8}Mn_2O_7$, for which a commensurate AFM correlation is observed in the paramagnetic insulating state [9]. If the electron density is relatively close to half-filling, the tendency to the FM state is suppressed. This assumption is also consistent with the recent numerical results [6,7]. In this case, it is plausible to assume the presence of the finite AFM correlation length ξ_{AFM}. Then, within the scale smaller than ξ_{AFM}, we can put $\vec{m} = e^{-i\pi j}\vec{n}$ with $\vec{n}$ a unit vector. By substituting the above expression into the action, we get from the J_H term the following expression :

$$(\vec{J_L} + \vec{J_R})\cdot\vec{l_j} + (\mathrm{Tr}(g\vec{\sigma})e^{i\sqrt{2\pi}\phi_c}e^{(2k_F-\pi)x} + h.c.)\sqrt{1-l^2}\vec{n} + (\vec{J_L} + \vec{J_R})\sqrt{1-l^2}e^{-i\pi x}\vec{n} + (\mathrm{Tr}(g\vec{\sigma})e^{i2k_Fx}e^{i\sqrt{2\pi}\phi_c} + h.c.)\vec{l}. \quad (5)$$

The first term proportional to $\vec{l}$ which carries the fluctuations of the spin configuration coupled with the degrees of freedom of the conduction electron is not important for the transport properties which are of primary concern, since it does not couple to the charge degrees of freedom. The last two terms which contain the rapidly oscillating factor give subdominant contributions. The second, proportional to $\vec{n}$ term is predominant and is going to generate a gap. In order to deal with this term, we follow the method developed by Tsvelik [12]. We first neglect the fast variable and approximate $\sqrt{1-l^2} \simeq 1$. The effect of the fast variable will be considered later. By writing $i\vec{\sigma}\cdot\vec{n} \equiv h \in \mathrm{SU}(2)$ and subsequently $gh \equiv G$ this term is transformed to :

$$(\mathrm{Tr}(G)e^{i\sqrt{2\pi}\phi_c}e^{i(2k_F-\pi)x} + h.c.). \quad (6)$$

By refermionizing the above expression we get $\mathrm{Tr}(G)e^{i\sqrt{2\pi}\phi_c} = {\psi_{R,\alpha}}^\dagger\psi_{L,\alpha}$ where summation over spin indices is assumed. Then the part of the action which involves only the degrees of freedom of the conduction electron, together with the above term can be refermionized into the form :

$$S_0 = \int dxd\tau[v{\psi_{R,\alpha}}^\dagger\partial\psi_{R,\alpha} - v{\psi_{L,\alpha}}^\dagger\partial\psi_{L,\alpha} + J_HS{\psi_{R,\alpha}}^\dagger\psi_{L,\alpha}e^{i\delta x} + h.c.] \quad (7)$$

We have defined $\delta = 2k_F - \pi$. The diagonalization of the above Hamiltonian is an easy task giving the dispersion relation : $\epsilon_k = \pm\sqrt{v^2k^2 + {J_H}^2S^2} - v\delta/2$. The important feature of the above analysis is that when $J_HS \geq v\delta/2$ a massive state with a gap $\Delta = J_HS - v|\delta|/2$ appears despite the fact that an oscillatory factor exists in the crossed term of Eq.(7). In this massive state, we should interpret $v|\delta|/2$ as a chemical potential which lies within the gap. The strong correlation between the gap and the distance from half-filling is remarkable. In principle if $J_HS > v|\delta|/2$ there is always a gap in the spectrum. Note that our approach is non-perturbative in J_HS/v. This argument is consistent under the condition that the local AFM correlation length is large enough to produce the mass gap; *i.e.* $\Delta^{-1} < \xi_{\mathrm{AFM}}$. Following ref. [14], we can show that the spin degrees of freedom are described in terms of an $O(3)$ nonlinear σ model without the topological term. If the relation $J_{AFM} \gg J_H^2/v$, which is the condition for the presence of local AFM fluctuations, holds, the mass gap of the spin excitation is given by

$\sim \exp(-\pi S)$. Thus for sufficiently large S, the above condition, $\Delta^{-1} < \xi_{\rm AFM}$, is satisfied, and our argument is applicable. Note that the gap Δ is not a function of J_{AFM} but only of J_H and δ. The direct AFM term is physically needed to ensure the existence of the PM state in the form of short AFM correlations (even away from half - filling).

The dc conductivity for this state can be easily computed using the Kubo formula (current-current correlation) and we have the expression for the resistivity: $\rho \propto e^{\Delta/kT}$ for $kT \ll \Delta$. The physics behind these calculations is that in the paramagnetic state the strong AFM fluctuations are able to form bound states between the localized spins and the conduction electrons, leading to a gap generation [14]. The only possibility to achieve non-zero conductivity is through temperature fluctuations which can "break" these bound states. The insulating state is quite due to the frustration effect of the spin systems. The itinerant electrons give rise to the frustration between $2k_F$ RKKY interaction and the direct exchange interaction. In order to suppress this frustration, the localized state of electrons is favored energetically for sufficiently large J_H.

So far we have neglected the fast variable $\vec{l}$. Even if we include it, the above result is not changed essentially. After the gap formation, taking up to the second order in $\vec{l}$, we integrate out the fast variable. Then, we find that it just renormalizes the mass gap, and does not change the low-energy qualitative properties.

Ferromagnetic regime : Now let's consider the FM state. When δ increases, the gap Δ obtained in the vicinity of the half-filling collapses. This implies the backward scattering term of J_H term becomes irrelevant, and that the forward scattering term of J_H, which induces the FM fluctuation between localized spins, determines the low-energy physics, overcoming the AFM fluctuations due to the direct exchange interaction. This picture is again supported by the numerical results [6,7]. Although the FM state is realized for $J_H/t \gg 1$, in which case the bosonization approach is not applicable, we can stabilize the FM state for a small value of J_H/t by applying an external magnetic field as will be discussed later. Thus, here, we assume the presence of the FM order. In this case, we can parametrize $\vec{S} = S\vec{n} = S(\sin\varphi\cos\alpha, \cos\varphi\cos\alpha, \sin\alpha)$ in eq.(4), where the averaged magnetization in the FM state is assumed to be in the z-direction. The action which describes the spin wave is given by

$$S_{SW} = \int dx d\tau v_s [iS\alpha c^{-1}\partial_\tau\varphi + (\partial_x\varphi)^2 + (\partial_x\alpha)^2], \quad (8)$$

where c is a constant. The coupling between conduction electrons and the $\vec{n}$ field through J_H term is given by,

$$J_H(\vec{J_L} + \vec{J_R}) \cdot \vec{n} + J_H S(e^{i2k_F x}{\rm Tr}(g\vec{\sigma})e^{i\sqrt{2\pi}\phi_c} + h.c.) \cdot \vec{n}. \quad (9)$$

The second term of the above equation which involves the charge degrees of freedom contains a rapidly oscillating factor $\exp(2ik_F x)$. Thus, it is an irrelevant interaction at the low-energy fixed point, and the system is described in terms of free fermions in a magnetic field (Zeeman interaction) with the dispersion relation: $\epsilon_k = v|k| \pm J_H S$. There is no finite resistivity at this low-energy fixed point. The system is an ideal metal. Since in 1D systems the transition temperature to the FM state T_c is equal to zero, we can not discuss about the resistivity at finite temperatures in this framework. However, it is an instructive and interesting issue to consider the temperature dependence of the resistivity in this state assuming $T_c \neq 0$ due to some magnetic coupling with three-dimensional directions [16]. In this case, the second term of eq.(9) may give rise to the resistivity at finite temperatures. In order to see this, we calculate the resistivity using the memory function formalism, and treating the above term perturbatively as done by Giamarchi for the Sine-Gordon model [17]. This approach for the calculation of resistivity is followed with special care, because it gives a finite value even for 1D integrable systems, which are intrinsically ideal metals or ideal insulators [18]. However, since our system is not integrable, we expect that this method gives qualitatively correct temperature dependence of the resistivity. The lowest order non-vanishing contribution comes from the second order term in $J_H S$ after averaging over φ and α. The oscillating factors $\exp(\pm 4i(k_F/v)x)$ which appear in all terms involving the charge degrees of freedom determine the dominant temperature dependence of the resistivity. The result is given by $\rho \propto J_H^2 S^2 \exp(-a(k_F v)/T)$ with a a constant for $T \ll k_F v_F$. Although there is a prefactor which depends on the temperature, the dominant temperature dependence is determined by the exponential decay. Thus, the resistivity decreases very rapidly in the FM state as temperature decreases, and at zero temperature the system is an ideal metal with an infinite conductivity. This feature should be closely relevant to the colossal change of the resistance observed in oxide manganites.

Effect of an applied field: We now discuss the effect of an external field H_0 ($> H_c$) which is a direct extension of the FM case. The qualitative argument for this statement can be understood in two basic steps. In the first place the application of a field is going to reduce the effect of the antiferromagnetic fluctuations and (through a Zeeman term) to produce a non-zero average - both in time and space - magnetization of the localized spins towards the preferred direction. The second step is that through the strong J_H term the "effective field" which affects the conduction electron is enhanced by the factor J_H and is much stronger. Therefore our calculations (definitely in the FM regime for $\mu H_0 > J_{AFM} S^2$, μ

the magnetization of the localized spins) indicate again that the two bands split and the energy difference is exactly what has been found in the FM case enhanced by 2 $\vec{\mu} \cdot \vec{H}_{eff} = 2\mu H_{eff}$, where here μ is the magnetization of the conduction electrons. The application of an external field therefore largely contributes to the increase of the conductivity as observed in all the experimental data. A more detailed study of the crossover and the existence the critical field H_c above which the FM behavior is obtained, is a different issue that will be reported elsewhere. The basic question that has to be addressed, in order to give a full answer of this specific problem, is the precise effect of the field in the renormalization of the mass gap in the paramagnetic state or equivalently to take into account the intermediate states from the PM to FM.

In summary, we have analyzed the transport properties of the 1D FM Kondo Model with AFM fluctuations in two different regimes of the phase diagram, discovering an almost insulating behavior in the paramagnetic case and an almost zero resistivity in the FM case. As a general conclusion of these non-perturbative calculations we would like to stress the interplay - by purely magnetic interactions - between the ordered and the paramagnetic state. The very fact that numerical calculations in the model are able to demonstrate the existence of similar phases both in 1d and in higher dimensions, in agreement with the available experimental data, serves as a strong indication that the model and the results are relevant to the CMR problem. Since in 1D there is not an actual phase transition at finite temperatures, we lack a detailed description relevant to the temperature range in the vicinity of the actual T_c (besides the totally different behavior in the two regimes that has been discussed). The physical picture we would like to emphasize though, is that given a fixed set of *appropriate* interaction parameters and filling, the system can be in the FM or in the PM regime as a function of temperature, with the consequences described above which are qualitatively very close to the experimental findings. Therefore, the basic idea of this mechanism can be extended to more than 1D and, in addition to the strong electron-lattice coupling or other mechanisms (which are of secondary importance in this approach), may explain the dramatic dependence of the resistivity on the temperature.

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